

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1			Web Page for STN Seminar Schedule - N. America
NEWS	2	NOV	21	CAS patent coverage to include exemplified prophetic substances identified in English-, French-, German-, and Japanese-language basic patents from 2004-present
NEWS	3	NOV	26	MARPAT enhanced with FSORT command
NEWS	4	NOV	26	CHEMSAFE now available on STN Easy
NEWS	5	NOV	26	Two new SET commands increase convenience of STN searching
NEWS	6	DEC	01	ChemPort single article sales feature unavailable
NEWS	7	DEC	12	GBFULL now offers single source for full-text coverage of complete UK patent families
NEWS	8	DEC	17	Fifty-one pharmaceutical ingredients added to PS
NEWS	9	JAN	06	The retention policy for unread STNmail messages will change in 2009 for STN-Columbus and STN-Tokyo
NEWS	10	JAN	07	WPIDS, WPINDEX, and WPIX enhanced Japanese Patent Classification Data
NEWS	11	FEB	02	Simultaneous left and right truncation (SLART) added for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS	12	FEB	02	GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS	13	FEB	06	Patent sequence location (PSL) data added to USGENE
NEWS	14	FEB	10	COMPENDEX reloaded and enhanced
NEWS	15	FEB	11	WTEXTILES reloaded and enhanced
NEWS	16	FEB	19	New patent-examiner citations in 300,000 CA/CAPLUS patent records provide insights into related prior art
NEWS	17	FEB	19	Increase the precision of your patent queries -- use terms from the IPC Thesaurus, Version 2009.01
NEWS	18	FEB	23	Several formats for image display and print options discontinued in USPATFULL and USPAT2
NEWS	19	FEB	23	MEDLINE now offers more precise author group fields and 2009 MeSH terms
NEWS	20	FEB	23	TOXCENTER updates mirror those of MEDLINE - more precise author group fields and 2009 MeSH terms
NEWS	21	FEB	23	Three million new patent records blast AEROSPACE into STN patent clusters
NEWS	22	FEB	25	USGENE enhanced with patent family and legal status display data from INPADOCDB
NEWS	23	MAR	06	INPADOCDB and INPAFAMDB enhanced with new display formats
NEWS	24	MAR	11	EPFULL backfile enhanced with additional full-text applications and grants
NEWS	25	MAR	11	ESBIOBASE reloaded and enhanced
NEWS	26	MAR	20	CAS databases on STN enhanced with new super role for nanomaterial substances
NEWS	27	MAR	23	CA/CAPLUS enhanced with more than 250,000 patent equivalents from China

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,  
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS      STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN      Welcome Banner and News Items  
NEWS IPC8        For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 11:07:59 ON 24 MAR 2009

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.44	0.44

FILE 'REGISTRY' ENTERED AT 11:08:59 ON 24 MAR 2009

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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STRUCTURE FILE UPDATES: 22 MAR 2009 HIGHEST RN 1125392-64-4

DICTIONARY FILE UPDATES: 22 MAR 2009 HIGHEST RN 1125392-64-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.48	0.92

FILE 'REGISTRY' ENTERED AT 11:09:43 ON 24 MAR 2009

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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STRUCTURE FILE UPDATES: 22 MAR 2009 HIGHEST RN 1125392-64-4  
DICTIONARY FILE UPDATES: 22 MAR 2009 HIGHEST RN 1125392-64-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

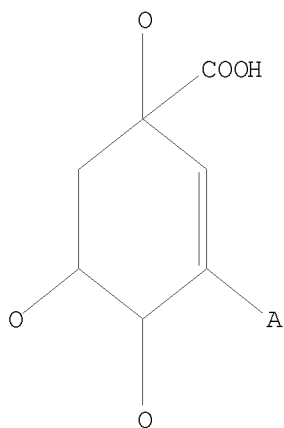
Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary  
files\10565348\10565348 RCE core.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam

SAMPLE SEARCH INITIATED 11:11:20 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 255 TO ITERATE

100.0% PROCESSED 255 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 4142 TO 6058

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> search l1 sss full  
FULL SEARCH INITIATED 11:11:40 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 5060 TO ITERATE

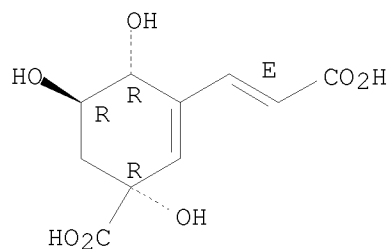
100.0% PROCESSED 5060 ITERATIONS 18 ANSWERS  
SEARCH TIME: 00.00.01

L3 18 SEA SSS FUL L1

=> d scan

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Cyclohexene-1-carboxylic acid, 3-[(1E)-2-carboxyethenyl]-1,4,5-  
trihydroxy-, (1R,4R,5R)-  
MF C10 H12 O7

Absolute stereochemistry.  
Double bond geometry as shown.

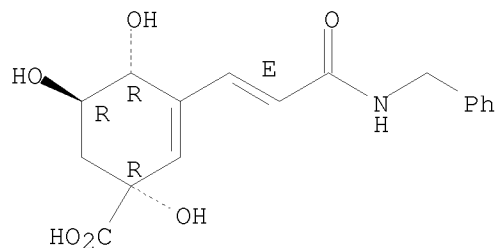


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):18

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-oxo-3-  
[(phenylmethyl)amino]-1-propen-1-yl]-, (1R,4R,5R)-  
MF C17 H19 N O6

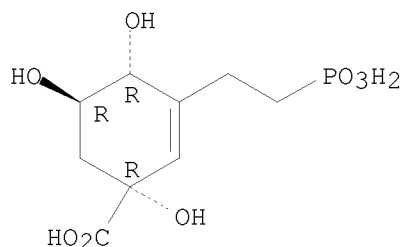
Absolute stereochemistry. Rotation (-).  
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-(2-phosphonoethyl)-,  
(1R,4R,5R)-  
MF C9 H15 O8 P

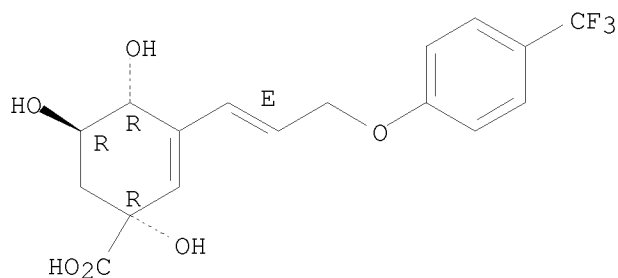
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-[4-(trifluoromethyl)phenoxy]-1-propen-1-yl]-, (1R,4R,5R)-  
MF C17 H17 F3 O6

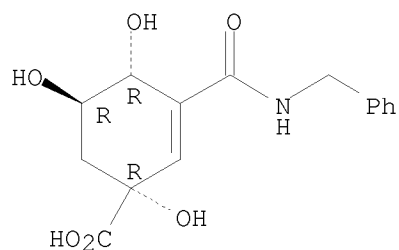
Absolute stereochemistry.  
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-  
[[ (phenylmethyl)amino]carbonyl]-, (1R,4R,5R)-  
MF C15 H17 N O6

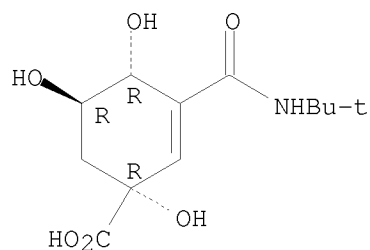
Absolute stereochemistry. Rotation (-).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2-Cyclohexene-1-carboxylic acid, 3-[[1,1-dimethylethyl]amino]carbonyl]-  
 1,4,5-trihydroxy-, (1R,4R,5R)-  
 MF C12 H19 N O6

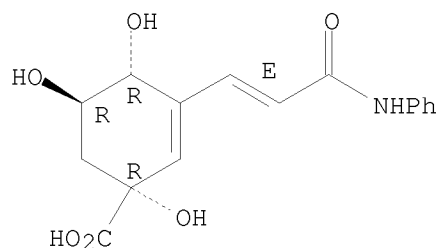
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-oxo-3-(  
 phenylamino)-1-propen-1-yl]-, (1R,4R,5R)-  
 MF C16 H17 N O6

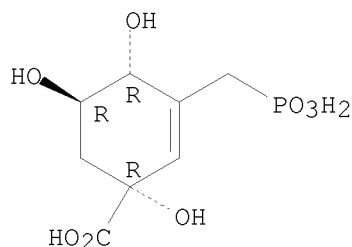
Absolute stereochemistry. Rotation (-).  
 Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-(phosphonomethyl)-,  
(1R,4R,5R)-  
MF C8 H13 O8 P

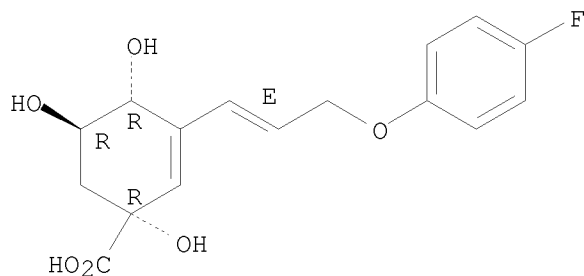
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Cyclohexene-1-carboxylic acid, 3-[(1E)-3-(4-fluorophenoxy)-1-propen-1-yl]-1,4,5-trihydroxy-, (1R,4R,5R)-  
MF C16 H17 F O6

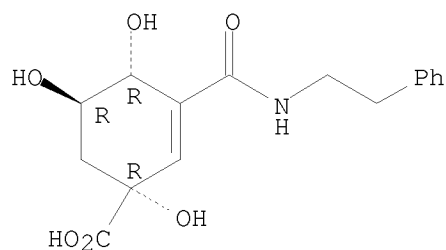
Absolute stereochemistry. Rotation (-).  
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[[2-phenylethyl)amino]carbonyl]-, (1R,4R,5R)-  
MF C16 H19 N O6

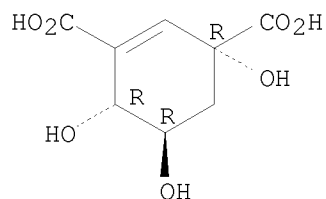
Absolute stereochemistry. Rotation (-).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1-Cyclohexene-1,3-dicarboxylic acid, 3,5,6-trihydroxy-, (3R,5R,6R)-  
 MF C8 H10 O7

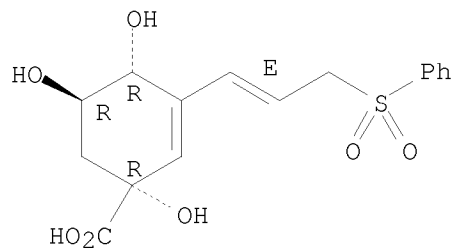
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-(phenylsulfonyl)-1-propen-1-yl]-, (1R,4R,5R)-  
 MF C16 H18 O7 S

Absolute stereochemistry. Rotation (-).  
 Double bond geometry as shown.



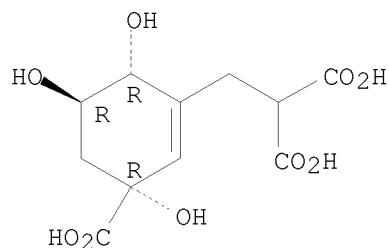
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN



IN Propanedioic acid, 2-[[ (3R,5R,6R)-3-carboxy-3,5,6-trihydroxy-1-cyclohexen-1-yl]methyl]-  
MF C11 H14 O9

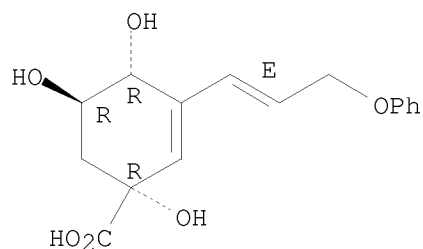
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-phenoxy-1-propen-1-yl]-, (1R,4R,5R)-  
MF C16 H18 O6

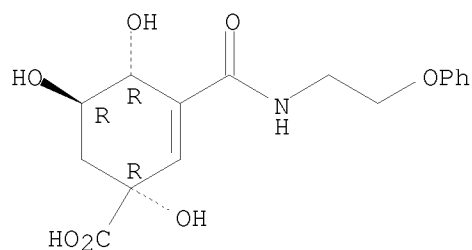
Absolute stereochemistry. Rotation (-).  
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[[ (2-phenoxyethyl)amino]carbonyl]-, (1R,4R,5R)-  
MF C16 H19 N O7

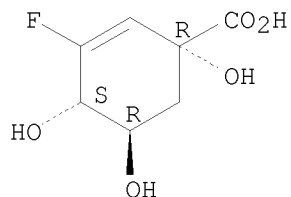
Absolute stereochemistry. Rotation (-).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-  
 MF C7 H9 F O5

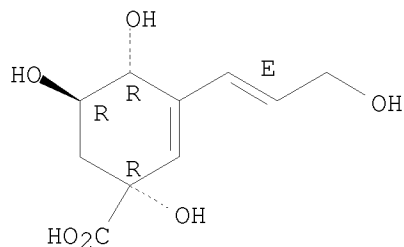
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-hydroxy-1-propen-1-yl]-, (1R,4R,5R)-  
 MF C10 H14 O6

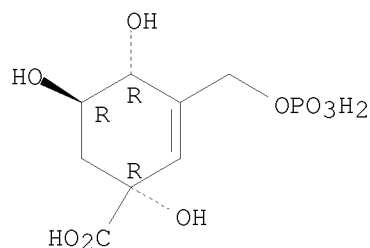
Absolute stereochemistry. Rotation (-).  
 Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(phosphonoxy)methyl]-  
, (1R,4R,5R)-  
MF C8 H13 O9 P

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
187.80	188.72

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 11:12:55 ON 24 MAR 2009  
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FILE COVERS 1907 - 24 Mar 2009 VOL 150 ISS 13  
FILE LAST UPDATED: 23 Mar 2009 (20090323/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

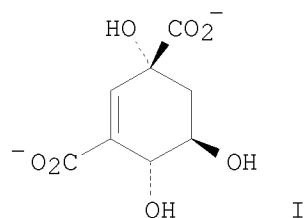
=> 13

L4 6 L3

=> d 14 1-6 ti fbib abs

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN  
TI Rational design, synthesis, and evaluation of nanomolar type II  
dehydroquinase inhibitors  
AN 2007:808773 CAPLUS <<LOGINID::20090324>>  
DN 147:268289  
TI Rational design, synthesis, and evaluation of nanomolar type II  
dehydroquinase inhibitors  
AU Payne, Richard J.; Peyrot, Fabienne; Kerbarh, Olivier; Abell, Andrew D.;  
Abell, Chris  
CS Department of Chemistry, University of Cambridge, Cambridge, CB2 1EW, UK  
SO ChemMedChem (2007), 2(7), 1015-1029  
CODEN: CHEMGX; ISSN: 1860-7179  
PB Wiley-VCH Verlag GmbH & Co. KGaA  
DT Journal  
LA English  
OS CASREACT 147:268289  
AB The in silico design, synthesis, and biol. evaluation of ten potent type  
II dehydroquinase inhibitors are described. These compds. contain an  
anhydroquinone core, incorporated as a mimic of the enolate reaction  
intermediate. This substructure is attached by a variety of linking units  
to a terminal Ph group that binds in an adjacent pocket. Inhibitors were  
synthesized from (-)-quinic acid using palladium-catalyzed Stille and  
carboamidation chemical. Several inhibitors exhibited nanomolar inhibition  
consts. against type II dehydroquinases from Streptomyces coelicolor and  
Mycobacterium tuberculosis. These are among the most potent inhibitors of  
these enzymes reported to date.  
RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN  
TI Nanomolar inhibition of type II dehydroquinase based on the enolate  
reaction mechanism  
AN 2007:341043 CAPLUS <<LOGINID::20090324>>  
DN 147:671  
TI Nanomolar inhibition of type II dehydroquinase based on the enolate  
reaction mechanism  
AU Toscano, Miguel D.; Payne, Richard J.; Chiba, Akira; Kerbarh, Olivier;  
Abell, Chris  
CS Department of Chemistry, University Chemical Laboratory, University of  
Cambridge, Cambridge, CB2 1EW, UK  
SO ChemMedChem (2007), 2(1), 101-112  
CODEN: CHEMGX; ISSN: 1860-7179  
PB Wiley-VCH Verlag GmbH & Co. KGaA  
DT Journal  
LA English  
OS CASREACT 147:671  
GI



AB The authors describe the rational design of a novel, highly potent inhibitor of type II dehydroquinase, the dicarboxylate (I). The incorporation of a carboxylate at the 3-position mimics the putative enolate intermediate in the reaction mechanism, and allows a potential electrostatic binding interaction with the arginine on the active site flap. This results in a 1000-fold increase in potency, making the dicarboxylate I the most potent inhibitor of type II dehydroquinase reported to date, with a high ligand efficiency of -0.68 kcal mol<sup>-1</sup> per nonhydrogen atom. The systematic dissection of I in compds. 7-12, all of which show a drop in potency, confirm the synergistic importance of the two carboxylates, the C3 and C4 hydroxyl groups, and the anhydroquinone ring structure for the potency of I.

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN

TI Hot off the press

AN 2004:746639 CAPLUS <<LOGINID::20090324>>

DN 142:350581

TI Hot off the press

AU Hill, Robert A.; Sutherland, Andrew

CS Department of Chemistry, Glasgow University, Glasgow, G12 8QQ, UK

SO Natural Product Reports (2004), 21(4), H13-H15

CODEN: NPRRDF; ISSN: 0265-0568

PB Royal Society of Chemistry

DT Journal; General Review

LA English

AB A review covering a selection of 36 recent papers is presented the examines various aspects of current developments in bioorg. chemical and novel natural products such as bielschowskyin which has a novel diterpenoid framework and shows antimalarial and anticancer activity.

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN

TI (1R,4S,5R)-3-Fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid: the fluoro analogue of the enolate intermediate in the reaction catalyzed by type II dehydroquinases

AN 2004:422880 CAPLUS <<LOGINID::20090324>>

DN 141:140692

TI (1R,4S,5R)-3-Fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid: the fluoro analogue of the enolate intermediate in the reaction catalyzed by type II dehydroquinases

AU Frederickson, Martyn; Roszak, Aleksander W.; Coggins, John R.; Lapthorn, Adrian J.; Abell, Chris

CS University Chemical Laboratory, Cambridge, CB2 1EW, UK

SO Organic & Biomolecular Chemistry (2004), 2(11), 1592-1596

CODEN: OBCRAK; ISSN: 1477-0520

PB Royal Society of Chemistry

DT Journal

LA English

OS CASREACT 141:140692

AB The fluoro analog of the enolate intermediate in the reaction catalyzed by type II dehydroquinases has been prepared from naturally occurring (-)-quinic acid over seven steps and has been shown to be the most potent inhibitor reported to date of the type II enzyme from Mycobacterium tuberculosis.

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN

TI Vinyl fluoride as an isoelectronic replacement for an enolate anion:  
Inhibition of type II dehydroquinases

AN 2002:647422 CAPLUS <<LOGINID::20090324>>

DN 138:102740

TI Vinyl fluoride as an isoelectronic replacement for an enolate anion:  
Inhibition of type II dehydroquinases

AU Frederickson, Martyn; Coggins, John R.; Abell, Chris

CS University Chemical Laboratory, Cambridge, CB2 1EW, UK

SO Chemical Communications (Cambridge, United Kingdom) (2002), (17),  
1886-1887

CODEN: CHCOFS; ISSN: 1359-7345

PB Royal Society of Chemistry

DT Journal

LA English

OS CASREACT 138:102740

AB A vinyl fluoride analog of the intermediate in the reaction catalyzed by type II dehydroquinase enzymes has been synthesized over seven steps from (-)-quinic acid and shown to be a potent enzyme inhibitor.

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN

TI Cyclohexenyl and Cyclohexylidene Inhibitors of 3-Dehydroquinase Synthase:  
Active Site Interactions Relevant to Enzyme Mechanism and Inhibitor Design

AN 1997:528717 CAPLUS <<LOGINID::20090324>>

DN 127:216861

OREF 127:42125a,42128a

TI Cyclohexenyl and Cyclohexylidene Inhibitors of 3-Dehydroquinase Synthase:  
Active Site Interactions Relevant to Enzyme Mechanism and Inhibitor Design

AU Montchamp, Jean-Luc; Frost, J. W.

CS Contribution from the Department of Chemistry, Michigan State University,  
East Lansing, MI, 48824, USA

SO Journal of the American Chemical Society (1997), 119(33), 7645-7653

CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

AB Cyclohexenyl and cyclohexylidene inhibitors possessing strategically placed olefinic residues, in general, bind to 3-dehydroquinase (DHQ) synthase more tightly than similarly substituted cyclohexyl inhibitors. All of the newly synthesized inhibitors were prepared from a common DHQ derivative. Cyclohexenyl phosphate 1 is the most potent inhibitor of DHQ synthase thus far identified with an inhibition constant ( $K_i = 1.2 \times 10^{-10}$  M), indicating active site binding 1000-fold tighter relative to the corresponding cyclohexyl phosphate 5. Cyclohexenyl tricarboxylate 2 binds 700-fold more tightly than similarly substituted cyclohexyl tricarboxylate 6 and is the first example of a nanomolar-level inhibitor ( $K_i = 8.6 \times 10^{-9}$  M) possessing neither a phosphate monoester or a phosphonic acid. Cyclohexenyl homophosphonate 4 ( $K_i = 3.0 \times 10^{-8}$  M) and cyclohexylidene homophosphonate 10 ( $K_i = 3.2 \times 10^{-9}$  M) bind 57- and 530-fold, resp., more tightly than the corresponding cyclohexyl

homophosphonate 8. Cyclohexylidene homophosphonate 10 is the first example of a nanomolar-level, homophosphonic acid inhibitor of DHQ synthase. Cyclohexylidene phosphonate 9 ( $K_i = 2.9 \times 10^{-10}$  M) is a 2.9-fold more potent inhibitor relative to cyclohexyl phosphonate 7 which was previously the most potent, slowly-reversible inhibitor of DHQ synthase. Cyclohexenyl phosphonate 3 ( $K_i = 1.2 \times 10^{-9}$  M) is the only olefin-containing, carbocyclic inhibitor where improved binding over the corresponding cyclohexyl analog was not observed. The impact of olefinic residues in inhibitors on active site binding may indicate that DHQ synthase plays an active catalytic role during Elcb elimination of inorg. phosphate from enzyme-bound substrate.

RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	31.50	220.22
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-4.92	-4.92

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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	31.50	220.22
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-4.92	-4.92

=> d 14 5 it

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN  
IT Enzyme kinetics  
(of inhibition; vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)  
IT Crystal structure  
(vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)  
IT 486430-86-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (crystal structure properties; vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)  
 IT 486430-83-5P  
 RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)  
 IT 77-95-2, (-)-Quinic acid 109-87-5 149-73-5 176798-33-7 227002-11-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)  
 IT 176798-26-8P 183474-88-6P 183475-04-9P 486430-85-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)  
 IT 486430-84-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)  
 IT 9012-66-2, E.C. 4.2.1.10  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (vinyl fluoride as an isoelectronic replacement for an enolate anion: inhibition of type II dehydroquinases)

=> 486430-83-5

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L6 3 L5

=> display hitstr l6 1-3

L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN

IT 486430-83-5

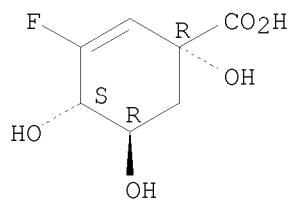
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (current developments in bioorg. chemical and novel natural products)

RN 486430-83-5 CAPLUS

CN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-  
 (CA INDEX NAME)

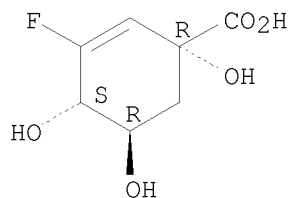
Absolute stereochemistry.





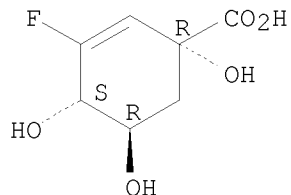
L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN  
 IT 486430-83-5P  
 RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);  
 BIOL (Biological study); PREP (Preparation)  
 (preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-  
 carboxylic acid analogs and their inhibition of bacterial  
 dehydroquinases)  
 RN 486430-83-5 CAPLUS  
 CN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-  
 (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN  
 IT 486430-83-5P  
 RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);  
 BIOL (Biological study); PREP (Preparation)  
 (vinyl fluoride analog as isoelectronic replacement for an enolate  
 anion and inhibitor of type II dehydroquinases)  
 RN 486430-83-5 CAPLUS  
 CN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-  
 (CA INDEX NAME)

Absolute stereochemistry.



=> logoff hold  
 COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST	ENTRY 11.16	SESSION 233.24
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-4.92

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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
FULL ESTIMATED COST	ENTRY 11.16	SESSION 233.24
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-4.92

=> d 14 3 it

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN

IT Natural products  
RL: BIOL (Biological study); OCCU (Occurrence); USES (Uses)  
(current developments in bioorg. chemical and novel natural products)

IT 10606-72-1P 128946-78-1P 178948-66-8P  
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP  
(Preparation)  
(current developments in bioorg. chemical and novel natural products)

IT 50-99-7, D-Glucose, biological studies 1603-79-8 71155-04-9  
72909-34-3, Pyrroloquinoline quinone 108605-69-2, Avenanthramide B  
486430-83-5 697299-12-0  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(current developments in bioorg. chemical and novel natural products)

IT 51532-30-0, (S)-4-Methyl-3-heptanone 149008-32-2,  
Phomacta-1(14),3,7-triene 689285-37-8, Mikamicranolide 694440-86-3,  
Clionastatin A 694440-87-4, Clionastatin B 701203-40-9, Corianlactone  
714954-37-7, Psymberin 719296-43-2, Carijenone 719298-06-3,  
Bisavenanthramide B 720681-08-3, Stolonilactone 720681-62-9,  
Oxaspirosuberitenone 720685-82-5, Sequosempervirin A 742088-25-1,  
Gymnorrhizol 790710-32-6, Spirodepressolide  
RL: BSU (Biological study, unclassified); NPO (Natural product  
occurrence); BIOL (Biological study); OCCU (Occurrence)  
(current developments in bioorg. chemical and novel natural products)

IT 697298-90-1, Bielschowskysin  
RL: BSU (Biological study, unclassified); NPO (Natural product  
occurrence); PAC (Pharmacological activity); PRP (Properties); THU

(Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)  
 (current developments in bioorg. chemical and novel natural products)  
 IT 677025-48-8, Menisporopsin A 681456-07-5 682334-57-2,  
 Brasilienosphylllic acid A 725254-09-1, Abyssomicin C  
 RL: BSU (Biological study, unclassified); NPO (Natural product  
 occurrence); PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
 (Biological study); OCCU (Occurrence); USES (Uses)  
 (current developments in bioorg. chemical and novel natural products)  
 IT 339541-50-3, Prerapamycin 360555-98-2, Spongidepsin  
 RL: BSU (Biological study, unclassified); NPO (Natural product  
 occurrence); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)  
 (current developments in bioorg. chemical and novel natural products)

=> 486430-83-5

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

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L8 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN

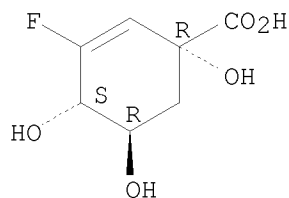
IT 486430-83-5

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (current developments in bioorg. chemical and novel natural products)

RN 486430-83-5 CAPLUS

CN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-  
 (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN

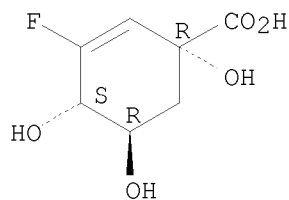
IT 486430-83-5P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);  
 BIOL (Biological study); PREP (Preparation)  
 (preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-  
 carboxylic acid analogs and their inhibition of bacterial  
 dehydroquinases)

RN 486430-83-5 CAPLUS

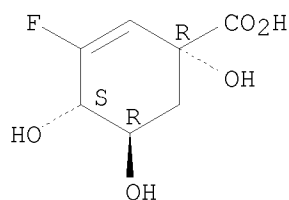
CN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-  
 (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN  
IT 486430-83-5P  
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);  
BIOL (Biological study); PREP (Preparation)  
(vinyl fluoride analog as isoelectronic replacement for an enolate  
anion and inhibitor of type II dehydroquinases)  
RN 486430-83-5 CAPLUS  
CN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-  
(CA INDEX NAME)

Absolute stereochemistry.



=> d 14 4 it

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN  
IT Cyclitols  
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);  
BIOL (Biological study); PREP (Preparation)  
(fluoro; preparation of  
(1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-  
carboxylic acid analogs and their inhibition of bacterial  
dehydroquinases)  
IT Mycobacterium tuberculosis  
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-  
carboxylic acid analogs and their inhibition of bacterial  
dehydroquinases)  
IT 9012-66-2  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-  
carboxylic acid analogs and their inhibition of bacterial  
dehydroquinases)  
IT 13019-10-8P 486430-83-5P 486430-84-6P  
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);  
BIOL (Biological study); PREP (Preparation)  
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-

carboxylic acid analogs and their inhibition of bacterial  
dehydroquinases)

IT 177284-79-6P 725738-25-0P  
RL: PNU (Preparation, unclassified); PREP (Preparation)  
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-  
carboxylic acid analogs and their inhibition of bacterial  
dehydroquinases)

IT 77-95-2, (-)-Quinic acid 177284-85-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-  
carboxylic acid analogs and their inhibition of bacterial  
dehydroquinases)

IT 176798-26-8P 183474-88-6P 183475-04-9P 486430-85-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-  
carboxylic acid analogs and their inhibition of bacterial  
dehydroquinases)

IT 177284-86-5P 177284-87-6P 486430-86-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-  
carboxylic acid analogs and their inhibition of bacterial  
dehydroquinases)

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
13.54	249.14

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-4.92

CA SUBSCRIBER PRICE

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